



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:46 AM UTC

PDB ID : 2X2R / pdb_00002x2r
Title : Crystal structure of human kinesin Eg5 in complex with (R)-2-amino-3-((4-chlorophenyl)diphenylmethylthio)propanoic acid
Authors : Kaan, H.Y.K.; Weiss, J.; Menger, D.; Ulaganathan, V.; Laggner, C.; Popowycz, F.; Joseph, B.; Kozielski, F.
Deposited on : 2010-01-15
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

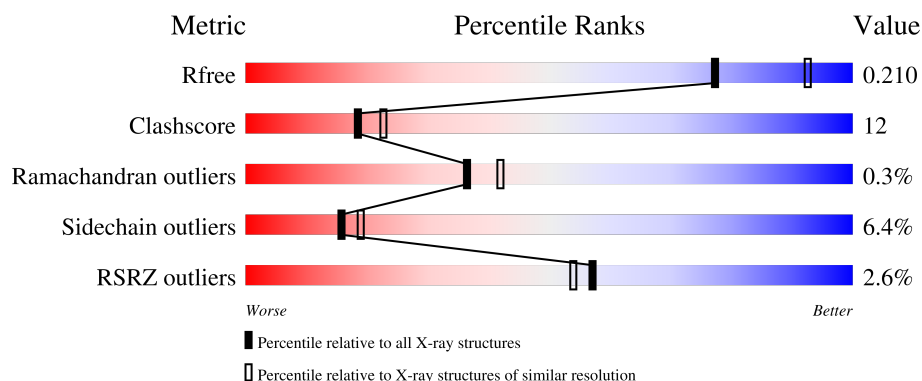
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	2% 69% 19% • 10%
1	B	368	2% 70% 14% • 12%
1	C	368	2% 64% 22% • • 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8687 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called KINESIN-LIKE PROTEIN KIF11.

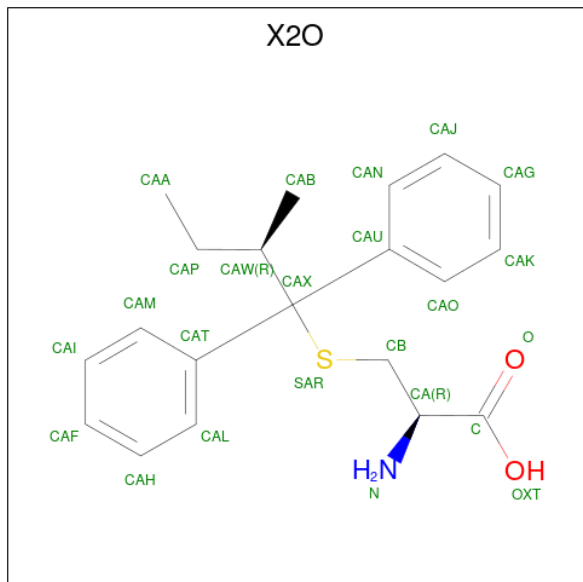
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	5	0
			2616	1641	452	512	11			
1	B	324	Total	C	N	O	S	0	10	0
			2588	1626	449	502	11			
1	C	329	Total	C	N	O	S	0	4	0
			2590	1624	447	509	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is (2R)-2-AMINO-3-[(2R)-2-METHYL-1,1-DIPHENYL-BUTYL]SULFANYL-PROPANOIC ACID (CCD ID: X2O) (formula: C₂₀H₂₅NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	20	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			24	20	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			24	20	1	2	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

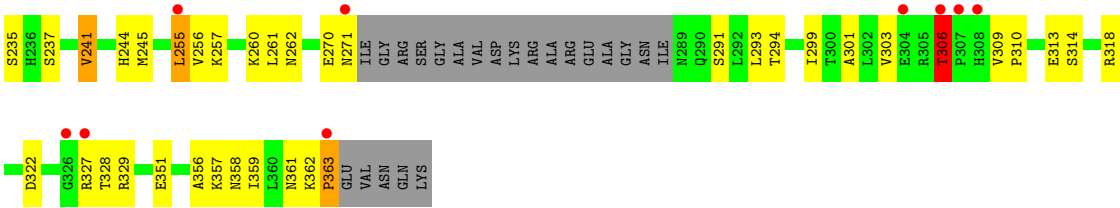
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total	O	0	0
			282	282		
5	B	283	Total	O	0	0
			283	283		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	172	Total	O	0	0
			172	172		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.35Å 96.35Å 124.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.41 – 2.20 29.41 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.41-2.20) 99.9 (29.41-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.172 , 0.216 0.169 , 0.210	Depositor DCC
R_{free} test set	3321 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.027 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8687	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: X2O, MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/2670	0.83	2/3611 (0.1%)
1	B	0.56	0/2655	0.81	1/3589 (0.0%)
1	C	0.52	1/2641 (0.0%)	0.82	2/3573 (0.1%)
All	All	0.55	1/7966 (0.0%)	0.82	5/10773 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	PRO	C-O	-5.52	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	THR	CA-C-N	5.77	124.97	118.97
1	C	306	THR	C-N-CA	5.77	124.97	118.97
1	B	308	HIS	N-CA-C	5.33	117.32	107.73
1	A	191	LYS	N-CA-C	5.30	118.85	112.38
1	A	122	ASN	N-CA-C	-5.29	99.53	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2651	58	0
1	B	2588	0	2643	61	0
1	C	2590	0	2614	70	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
3	A	24	0	24	2	0
3	B	24	0	24	1	0
3	C	24	0	24	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	282	0	0	9	0
5	B	283	0	0	6	0
5	C	172	0	0	6	0
All	All	8687	0	8016	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:O	1:B:363:PRO:CB	1.88	1.21
1:B:327:ARG:O	1:B:363:PRO:HB3	1.05	1.18
1:B:362:LYS:H	1:B:363:PRO:HD3	1.07	1.15
1:C:362:LYS:CB	1:C:363:PRO:HD3	1.80	1.10
1:B:327:ARG:HG3	1:B:363:PRO:HA	1.42	1.00
1:B:361:ASN:O	1:B:362:LYS:HD2	1.65	0.94
1:C:70:MET:HE1	1:C:84:SER:HB2	1.47	0.94
1:B:362:LYS:N	1:B:363:PRO:HD3	1.84	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:LYS:HB3	1:C:363:PRO:HD3	1.54	0.89
1:C:270:GLU:O	1:C:271:ASN:HB2	1.70	0.88
1:C:362:LYS:HB2	1:C:363:PRO:HD3	1.55	0.88
1:C:363:PRO:O	1:C:363:PRO:HG2	1.74	0.86
1:B:306:THR:HB	1:B:307:PRO:HD2	1.59	0.84
1:B:327:ARG:C	1:B:363:PRO:HB3	2.03	0.83
1:B:362:LYS:H	1:B:363:PRO:CD	1.90	0.82
1:B:239:PHE:HE1	1:B:241:VAL:HG22	1.44	0.81
1:B:361:ASN:O	1:B:362:LYS:CG	2.30	0.80
1:C:92:GLU:HG3	1:C:329:ARG:HH11	1.47	0.80
1:B:361:ASN:O	1:B:362:LYS:CD	2.30	0.79
1:A:95:MET:HE2	1:A:95:MET:HA	1.65	0.78
1:B:327:ARG:HG3	1:B:363:PRO:CA	2.13	0.78
1:B:361:ASN:O	1:B:362:LYS:CB	2.31	0.78
1:C:362:LYS:CB	1:C:363:PRO:CD	2.63	0.77
1:B:323:SER:HA	1:B:328:THR:HB	1.67	0.76
1:C:363:PRO:O	1:C:363:PRO:CG	2.30	0.74
1:C:245:MET:HE3	1:C:257:LYS:HG3	1.70	0.73
1:A:364:GLU:O	1:A:365:VAL:HG22	1.87	0.73
1:A:157:LYS:HE3	1:A:201:GLU:OE1	1.89	0.72
1:C:47:ARG:HH22	1:C:363:PRO:CD	2.02	0.72
1:C:226:THR:HG22	1:C:227:LEU:HD13	1.71	0.72
1:B:260:LYS:HE2	1:B:262:ASN:HD21	1.54	0.72
1:A:247:GLU:HG2	1:A:255:LEU:HG	1.72	0.71
1:C:235:SER:O	5:C:2127:HOH:O	2.09	0.70
1:C:293:LEU:HD12	1:C:294:THR:N	2.07	0.69
1:B:329:ARG:HG2	1:B:363:PRO:HG3	1.74	0.69
1:C:184:MET:HE3	1:C:318:ARG:NH1	2.09	0.68
1:C:184:MET:HE3	1:C:318:ARG:CZ	2.23	0.67
1:A:96:GLY:O	1:A:365:VAL:HB	1.95	0.67
1:A:87[B]:CYS:HB3	1:A:88:PRO:HD3	1.76	0.67
1:A:235:SER:O	5:A:2209:HOH:O	2.14	0.66
1:C:70:MET:HE1	1:C:84:SER:CB	2.24	0.65
1:C:146:LYS:O	1:C:150:ASN:HB2	1.96	0.65
1:A:327:ARG:O	1:A:363:PRO:HA	1.96	0.64
1:B:361:ASN:ND2	5:B:2272:HOH:O	2.30	0.62
1:A:364:GLU:O	1:A:365:VAL:CG2	2.47	0.62
1:B:87[A]:CYS:HB2	1:B:88:PRO:HD3	1.82	0.61
1:B:239:PHE:CE1	1:B:241:VAL:HG22	2.32	0.61
1:B:361:ASN:O	1:B:362:LYS:HB2	2.00	0.60
1:C:362:LYS:HB2	1:C:363:PRO:CD	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:HD22	1:C:357:LYS:HE3	1.67	0.58
1:C:47:ARG:NH2	1:C:363:PRO:HD2	2.18	0.58
1:B:29:ASN:O	1:B:33:ARG:HG3	2.03	0.58
1:A:82:TYR:CD2	1:A:86:VAL:HB	2.38	0.58
1:C:139:THR:HG21	1:C:261:LEU:HD23	1.87	0.57
1:B:119:ARG:HH21	1:B:130:ASP:HB2	1.70	0.56
1:C:66:TYR:OH	1:C:351:GLU:OE2	2.21	0.56
1:C:119:ARG:HH21	1:C:130:ASP:HB2	1.70	0.56
1:A:17:LYS:HE3	5:A:2001:HOH:O	2.04	0.56
1:B:236:HIS:CD2	1:B:267:ALA:H	2.24	0.56
1:C:47:ARG:HH22	1:C:363:PRO:HD2	1.69	0.55
1:C:152:THR:O	1:C:152:THR:HG23	2.04	0.55
1:A:289:ASN:N	5:A:2228:HOH:O	2.39	0.55
1:B:322:ASP:O	1:B:326:GLY:HA3	2.07	0.54
1:A:221:ARG:HD2	5:A:2210:HOH:O	2.08	0.54
1:C:152:THR:O	1:C:152:THR:CG2	2.57	0.53
1:C:98:ASN:ND2	1:C:260:LYS:HB3	2.24	0.52
3:C:1367:X2O:CAL	3:C:1367:X2O:HAB2	2.40	0.52
1:B:87[B]:CYS:HB3	1:B:88:PRO:HD3	1.90	0.52
1:A:60:LYS:HE3	5:A:2057:HOH:O	2.09	0.52
1:B:329:ARG:HG2	1:B:363:PRO:CG	2.40	0.52
1:C:301:ALA:HA	1:C:306:THR:HG23	1.90	0.52
1:A:102:PHE:HB3	1:A:264:VAL:HB	1.92	0.52
1:B:248:THR:HA	1:B:249:THR:C	2.35	0.51
1:A:56:GLY:O	1:A:60:LYS:HE2	2.10	0.51
1:B:102:PHE:HB3	1:B:264:VAL:HB	1.91	0.51
1:A:58:ALA:O	1:B:197:LYS:HD2	2.11	0.50
1:C:223:THR:O	1:C:226:THR:HB	2.11	0.50
1:A:121:PRO:O	1:A:122:ASN:HB2	2.11	0.50
1:A:44:ASP:OD2	1:A:47:ARG:HD2	2.12	0.49
1:C:158:VAL:HG12	1:C:241:VAL:HG13	1.94	0.49
1:A:30:LEU:HD23	1:A:34:LYS:HE2	1.93	0.49
1:C:270:GLU:O	1:C:271:ASN:CB	2.49	0.49
1:A:364:GLU:C	1:A:365:VAL:CG2	2.84	0.49
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.94	0.49
1:A:121:PRO:C	1:A:122:ASN:O	2.50	0.49
1:B:29:ASN:HB3	5:B:2276:HOH:O	2.13	0.49
1:C:161:LEU:HD12	1:C:161:LEU:C	2.39	0.48
1:A:189:ARG:HD2	5:A:2161:HOH:O	2.14	0.48
1:B:362:LYS:N	1:B:363:PRO:CD	2.58	0.48
1:A:82:TYR:CE2	1:A:86:VAL:HG11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLN:O	1:B:324:LEU:O	2.32	0.48
1:A:197:LYS:HD3	1:A:197:LYS:HA	1.51	0.48
1:B:157:LYS:HB2	1:B:157:LYS:HE2	1.49	0.48
1:A:116:GLU:HG2	1:A:136:ILE:HD12	1.96	0.47
1:C:27:PRO:HG3	1:C:74:ALA:O	2.14	0.47
1:B:121:PRO:HD2	5:B:2119:HOH:O	2.14	0.47
1:B:236:HIS:HE1	5:B:2235:HOH:O	1.97	0.47
1:A:255:LEU:HD23	1:A:255:LEU:N	2.29	0.47
1:A:116:GLU:OE1	1:A:221:ARG:NH2	2.47	0.47
1:C:68:PHE:HA	1:C:359:ILE:HD12	1.97	0.47
1:B:307:PRO:HG2	1:B:308:HIS:H	1.79	0.47
1:C:329:ARG:HA	5:C:2002:HOH:O	2.15	0.47
3:C:1367:X2O:HAB2	3:C:1367:X2O:HAL	1.97	0.47
1:B:323:SER:HA	1:B:328:THR:CB	2.43	0.47
1:C:309:VAL:HA	1:C:310:PRO:HD3	1.52	0.46
1:A:365:VAL:HG23	5:A:2099:HOH:O	2.14	0.46
1:B:223:THR:O	1:B:226:THR:HB	2.15	0.46
1:C:170:ASP:CG	1:C:173:ASN:HB2	2.41	0.46
1:A:303:VAL:O	1:A:305:ARG:NH1	2.49	0.46
1:C:90:LEU:O	1:C:94:ILE:HG12	2.16	0.46
1:A:152:THR:HG22	1:A:154:PHE:HB3	1.97	0.46
1:A:80:ASP:OD1	1:A:83:ARG:NH2	2.49	0.46
1:A:323:SER:HA	1:A:328:THR:HB	1.98	0.46
1:A:157:LYS:HE3	1:A:201:GLU:CD	2.41	0.45
1:B:327:ARG:CG	1:B:363:PRO:HA	2.31	0.45
1:A:152:THR:HG21	1:A:245:MET:HG2	1.99	0.45
1:C:72:PHE:CD1	1:C:76:THR:HG21	2.52	0.45
1:B:33:ARG:NE	5:B:2019:HOH:O	2.45	0.45
1:A:30:LEU:CD2	1:A:34:LYS:HE2	2.47	0.45
1:C:255:LEU:HD12	1:C:255:LEU:O	2.17	0.45
1:A:120:SER:HA	1:A:121:PRO:HD3	1.80	0.45
1:C:221:ARG:HD2	5:C:2128:HOH:O	2.16	0.45
1:A:87[A]:CYS:HB2	1:A:88:PRO:HD3	1.96	0.45
1:A:82:TYR:CE2	1:A:86:VAL:CG1	3.00	0.45
1:A:245:MET:HE3	1:A:245:MET:HB2	1.87	0.45
1:C:48:LYS:HB2	1:C:48:LYS:HE3	1.76	0.44
1:C:303:VAL:HG21	1:C:356:ALA:O	2.17	0.44
1:C:155:SER:HB3	1:C:244:HIS:HB2	1.98	0.44
1:C:116:GLU:OE1	1:C:221:ARG:NH2	2.49	0.44
1:B:291:SER:HA	1:B:314:SER:HB2	2.00	0.44
1:B:38:HIS:HD2	1:C:180:GLU:OE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG12	1:B:241:VAL:HG13	2.00	0.43
1:C:30:LEU:HD22	1:C:30:LEU:HA	1.84	0.43
1:A:365:VAL:CG2	5:A:2099:HOH:O	2.65	0.43
1:B:247:GLU:HB2	1:B:255:LEU:HD23	1.99	0.43
1:C:310:PRO:HB3	1:C:313:GLU:OE1	2.18	0.43
1:A:82:TYR:HE2	1:A:86:VAL:HG11	1.82	0.43
1:B:249:THR:O	1:B:255:LEU:HB2	2.19	0.43
1:A:85:VAL:O	1:A:89:ILE:HG12	2.18	0.43
1:B:20:GLN:OE1	1:B:70:MET:HE3	2.19	0.43
1:A:119:ARG:HG2	3:A:1367:X2O:HAP1	2.01	0.43
1:C:361:ASN:HA	5:C:2036:HOH:O	2.18	0.43
3:A:1367:X2O:HAB2	3:A:1367:X2O:CAL	2.48	0.43
1:C:178:VAL:HG22	1:C:178:VAL:O	2.19	0.43
1:A:206:ASN:OD1	1:A:208:ASP:HB2	2.19	0.42
1:B:361:ASN:HB3	1:B:363:PRO:HD3	2.00	0.42
3:B:1367:X2O:HAB2	3:B:1367:X2O:CAL	2.49	0.42
1:C:62:SER:O	1:C:63:ARG:HD3	2.19	0.42
1:A:355:ARG:NH1	5:A:2264:HOH:O	2.47	0.42
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.49	0.42
1:A:130:ASP:HA	1:A:131:PRO:HD3	1.95	0.42
1:A:314:SER:O	1:A:318:ARG:HG3	2.19	0.42
1:C:25:CYS:O	1:C:74:ALA:HA	2.20	0.42
1:C:184:MET:HE2	1:C:184:MET:HB3	1.86	0.42
1:B:55:GLY:HA3	1:B:59:ASP:O	2.20	0.42
1:C:136:ILE:HB	1:C:137:PRO:HD3	2.01	0.42
1:C:299:ILE:O	1:C:303:VAL:HG23	2.20	0.42
1:A:249:THR:HG22	1:A:253:GLU:H	1.85	0.42
1:C:106:GLN:HG2	1:C:109:THR:CG2	2.50	0.42
1:C:183:GLN:HG2	5:C:2045:HOH:O	2.20	0.42
1:C:100:THR:HG23	1:C:262:ASN:HB2	2.01	0.42
1:C:127:TRP:CE2	1:C:128[B]:GLU:HG3	2.54	0.42
1:B:17:LYS:HD3	1:B:17:LYS:HA	1.72	0.42
1:B:256:VAL:HG13	1:B:256:VAL:O	2.20	0.41
1:B:306:THR:HB	1:B:307:PRO:CD	2.41	0.41
1:C:291:SER:HA	1:C:314:SER:HB2	2.01	0.41
1:B:225:ALA:HA	1:B:231:TYR:HB3	2.02	0.41
1:B:264:VAL:HG12	1:B:266:LEU:HD13	2.02	0.41
1:C:92:GLU:OE2	1:C:329:ARG:HG3	2.19	0.41
1:B:207:LYS:NZ	5:B:2184:HOH:O	2.48	0.41
1:B:324:LEU:O	1:B:325:GLY:C	2.63	0.41
1:A:97:TYR:HA	1:A:365:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:HD2	1:A:322:ASP:OD1	2.20	0.41
1:B:361:ASN:O	1:B:362:LYS:HG3	2.19	0.41
1:C:120:SER:HA	1:C:121:PRO:HD2	1.88	0.41
1:C:18:ASN:N	5:C:2001:HOH:O	2.53	0.41
1:B:17:LYS:HD2	1:B:18:ASN:H	1.86	0.41
1:B:170:ASP:CG	1:B:173:ASN:HB2	2.46	0.41
1:C:291:SER:HA	1:C:314:SER:CB	2.50	0.41
1:A:168:LEU:HB2	1:A:182:LEU:HB2	2.02	0.41
1:C:134:GLY:O	1:C:137:PRO:HD2	2.21	0.41
1:A:187:ASP:OD1	1:A:189:ARG:HG2	2.20	0.41
1:A:364:GLU:C	1:A:365:VAL:HG23	2.45	0.41
1:B:147:LEU:HA	1:B:150[A]:ASN:HB2	2.03	0.41
1:B:189:ARG:H	1:B:189:ARG:HG3	1.64	0.41
1:C:173:ASN:HA	1:C:174:PRO:HD3	1.94	0.41
1:C:196:ILE:HG22	1:C:199:LEU:HB2	2.03	0.40
1:A:121:PRO:O	1:A:122:ASN:CB	2.64	0.40
1:C:64:LYS:HD2	1:C:64:LYS:HA	1.86	0.40
1:A:161:LEU:C	1:A:161:LEU:HD12	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/368 (90%)	326 (98%)	6 (2%)	0	100	100
1	B	327/368 (89%)	320 (98%)	5 (2%)	2 (1%)	21	23
1	C	329/368 (89%)	321 (98%)	7 (2%)	1 (0%)	36	42
All	All	988/1104 (90%)	967 (98%)	18 (2%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	ASN
1	B	362	LYS
1	C	152	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/322 (92%)	281 (94%)	17 (6%)	18	23
1	B	297/322 (92%)	278 (94%)	19 (6%)	16	19
1	C	294/322 (91%)	270 (92%)	24 (8%)	10	12
All	All	889/966 (92%)	829 (93%)	60 (7%)	16	17

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	52	VAL
1	A	123	GLU
1	A	124	GLU
1	A	128	GLU
1	A	197	LYS
1	A	212	GLN
1	A	220	LYS
1	A	227	LEU
1	A	246	LYS
1	A	254	GLU
1	A	255	LEU
1	A	297	ARG
1	A	306	THR
1	A	337	SER
1	A	364	GLU
1	A	365	VAL
1	B	17	LYS
1	B	19[A]	ILE
1	B	19[B]	ILE

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	150[A]	ASN
1	B	150[B]	ASN
1	B	157	LYS
1	B	165	ASN
1	B	189	ARG
1	B	191	LYS
1	B	226	THR
1	B	241	VAL
1	B	247	GLU
1	B	248	THR
1	B	249	THR
1	B	257	LYS
1	B	266	LEU
1	B	293	LEU
1	B	304	GLU
1	C	30	LEU
1	C	48	LYS
1	C	84	SER
1	C	92	GLU
1	C	119	ARG
1	C	124	GLU
1	C	128[A]	GLU
1	C	128[B]	GLU
1	C	146	LYS
1	C	152	THR
1	C	153	GLU
1	C	226	THR
1	C	227	LEU
1	C	237[A]	SER
1	C	237[B]	SER
1	C	241	VAL
1	C	255	LEU
1	C	256	VAL
1	C	306	THR
1	C	322	ASP
1	C	327	ARG
1	C	328	THR
1	C	358	ASN
1	C	363	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	141	HIS
1	A	321	GLN
1	A	358	ASN
1	B	38	HIS
1	B	205	HIS
1	B	236	HIS
1	B	262	ASN
1	B	321	GLN
1	B	361	ASN
1	C	18	ASN
1	C	38	HIS
1	C	98	ASN
1	C	150	ASN
1	C	183	GLN
1	C	262	ASN
1	C	321	GLN
1	C	358	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	1366	4	28,29,29	1.35	5 (17%)	43,45,45	1.84	9 (20%)
3	X2O	B	1367	-	22,25,25	0.75	0	24,34,34	0.96	2 (8%)
2	ADP	A	1366	4	28,29,29	1.40	3 (10%)	43,45,45	1.89	9 (20%)
3	X2O	A	1367	-	22,25,25	0.65	0	24,34,34	1.17	2 (8%)
3	X2O	C	1367	-	22,25,25	0.67	0	24,34,34	0.83	2 (8%)
2	ADP	B	1366	4	28,29,29	1.53	6 (21%)	43,45,45	1.85	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	1366	4	-	0/16/32/32	0/3/3/3
3	X2O	B	1367	-	-	0/28/30/30	0/2/2/2
2	ADP	A	1366	4	-	0/16/32/32	0/3/3/3
3	X2O	A	1367	-	-	0/28/30/30	0/2/2/2
3	X2O	C	1367	-	-	0/28/30/30	0/2/2/2
2	ADP	B	1366	4	-	0/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1366	ADP	C5-C4	4.98	1.48	1.39
2	A	1366	ADP	C5-C4	4.31	1.46	1.39
2	C	1366	ADP	C5-C4	4.17	1.46	1.39
2	A	1366	ADP	PA-O3A	3.24	1.63	1.59
2	A	1366	ADP	C5-C6	2.67	1.48	1.41
2	B	1366	ADP	C5-C6	2.66	1.48	1.41
2	C	1366	ADP	C5-N7	-2.66	1.34	1.39
2	B	1366	ADP	C5-N7	-2.62	1.34	1.39
2	B	1366	ADP	PA-O3A	2.48	1.62	1.59
2	C	1366	ADP	C5-C6	2.47	1.47	1.41
2	B	1366	ADP	C4-N9	-2.27	1.33	1.37
2	C	1366	ADP	C4-N9	-2.14	1.33	1.37
2	C	1366	ADP	C8-N9	-2.04	1.34	1.37
2	B	1366	ADP	C8-N9	-2.01	1.34	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1366	ADP	C5-C4-N3	-5.79	118.75	126.72
2	B	1366	ADP	C5-C4-N3	-5.49	119.16	126.72
2	C	1366	ADP	C5-C4-N3	-5.09	119.70	126.72
2	A	1366	ADP	N3-C4-N9	5.02	135.70	127.17
2	B	1366	ADP	N3-C4-N9	4.99	135.65	127.17
2	C	1366	ADP	N3-C4-N9	4.61	135.00	127.17
2	C	1366	ADP	N3-C2-N1	-3.94	122.62	128.58
2	A	1366	ADP	C2-N3-C4	3.80	121.11	111.83
2	C	1366	ADP	C4-N9-C8	3.78	109.70	105.74
2	B	1366	ADP	C4-N9-C8	3.63	109.55	105.74
3	A	1367	X2O	CAB-CAW-CAP	-3.55	107.26	110.83
2	C	1366	ADP	C2-N3-C4	3.49	120.35	111.83
2	A	1366	ADP	N3-C2-N1	-3.37	123.48	128.58
2	B	1366	ADP	C4-C5-N7	-3.33	106.78	110.58
2	A	1366	ADP	C4-N9-C8	3.33	109.23	105.74
2	B	1366	ADP	C2-N3-C4	3.27	119.82	111.83
2	B	1366	ADP	N3-C2-N1	-3.18	123.77	128.58
2	A	1366	ADP	C4-C5-N7	-3.17	106.96	110.58
2	C	1366	ADP	C4-C5-N7	-3.03	107.12	110.58
3	A	1367	X2O	CAA-CAP-CAW	-3.02	108.87	113.34
3	B	1367	X2O	CAA-CAP-CAW	-2.74	109.29	113.34
2	C	1366	ADP	C2-N1-C6	2.69	123.14	118.73
2	A	1366	ADP	C5-N7-C8	2.65	107.61	103.45
2	B	1366	ADP	C5-N7-C8	2.63	107.59	103.45
2	C	1366	ADP	C5-N7-C8	2.63	107.58	103.45
2	C	1366	ADP	N9-C8-N7	-2.56	110.30	113.94
3	C	1367	X2O	CAB-CAW-CAP	-2.40	108.42	110.83
3	B	1367	X2O	CAB-CAW-CAP	-2.35	108.47	110.83
2	B	1366	ADP	C2-N1-C6	2.34	122.58	118.73
2	A	1366	ADP	N9-C8-N7	-2.32	110.64	113.94
3	C	1367	X2O	CAA-CAP-CAW	-2.28	109.97	113.34
2	A	1366	ADP	C6-C5-N7	2.23	136.38	132.09
2	B	1366	ADP	N9-C8-N7	-2.14	110.89	113.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

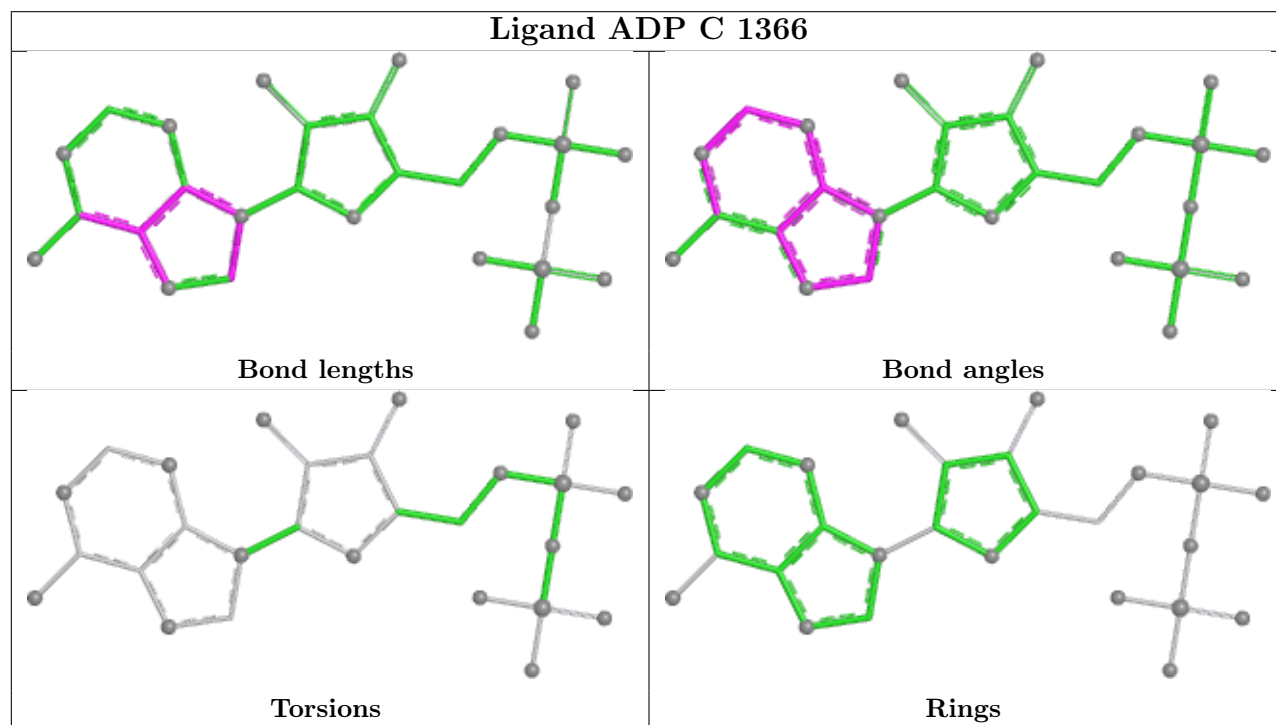
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1367	X2O	1	0
3	A	1367	X2O	2	0

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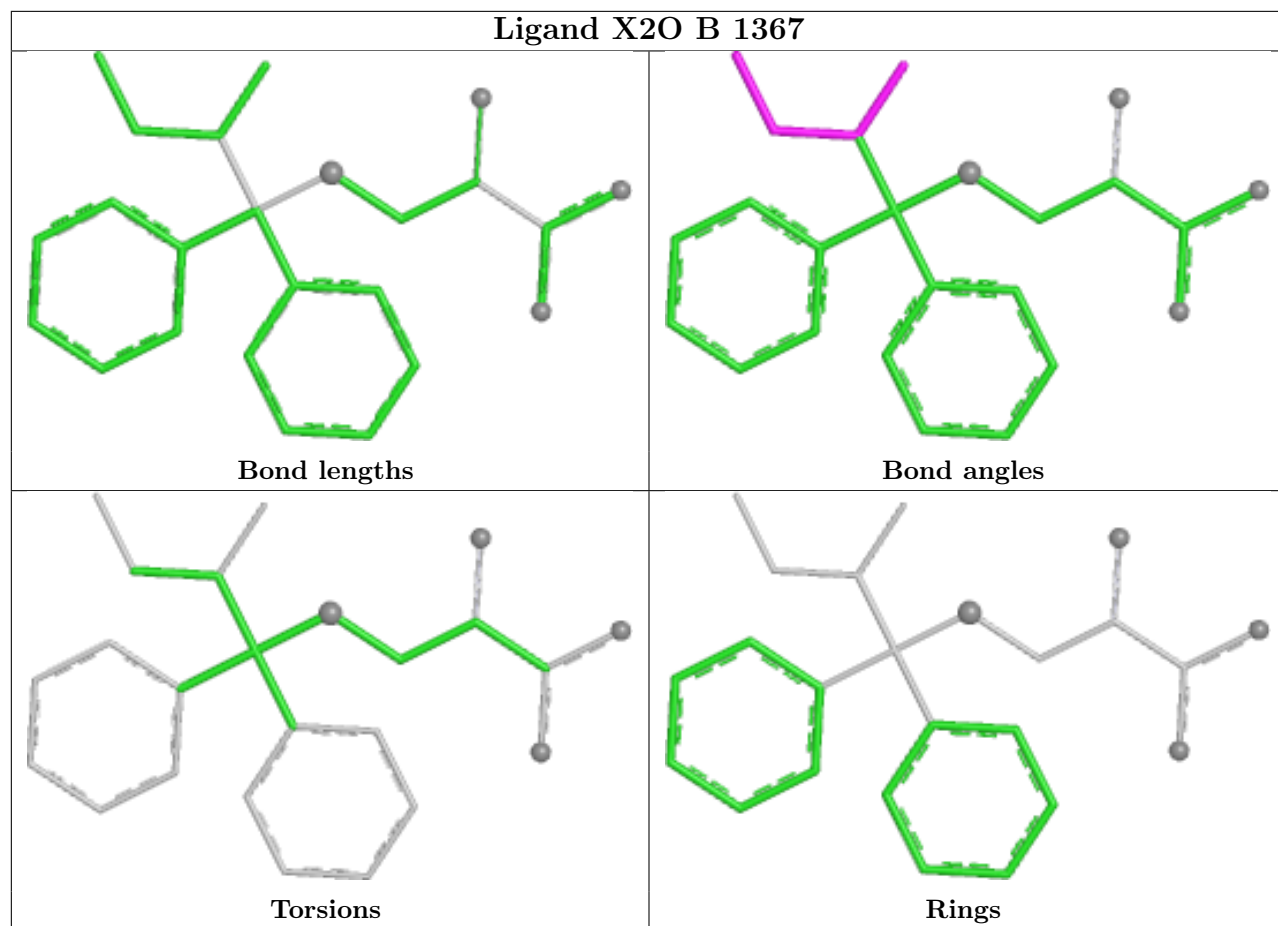
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1367	X2O	2	0

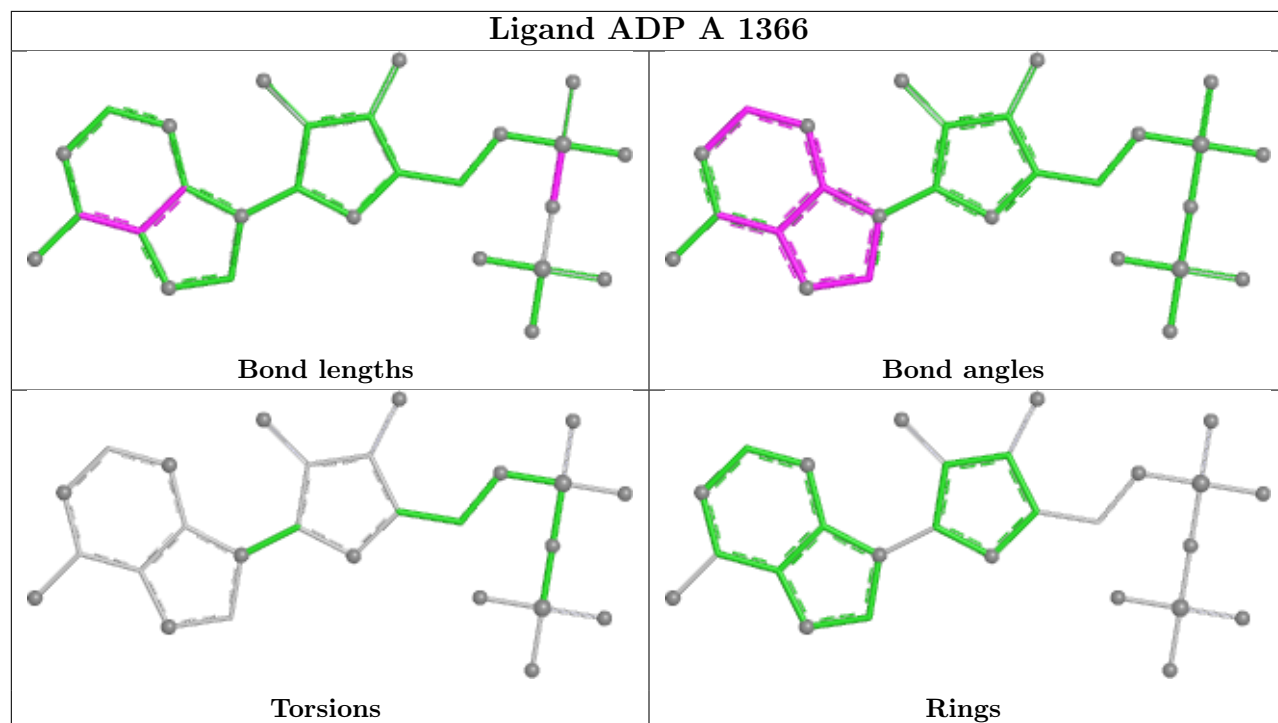
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

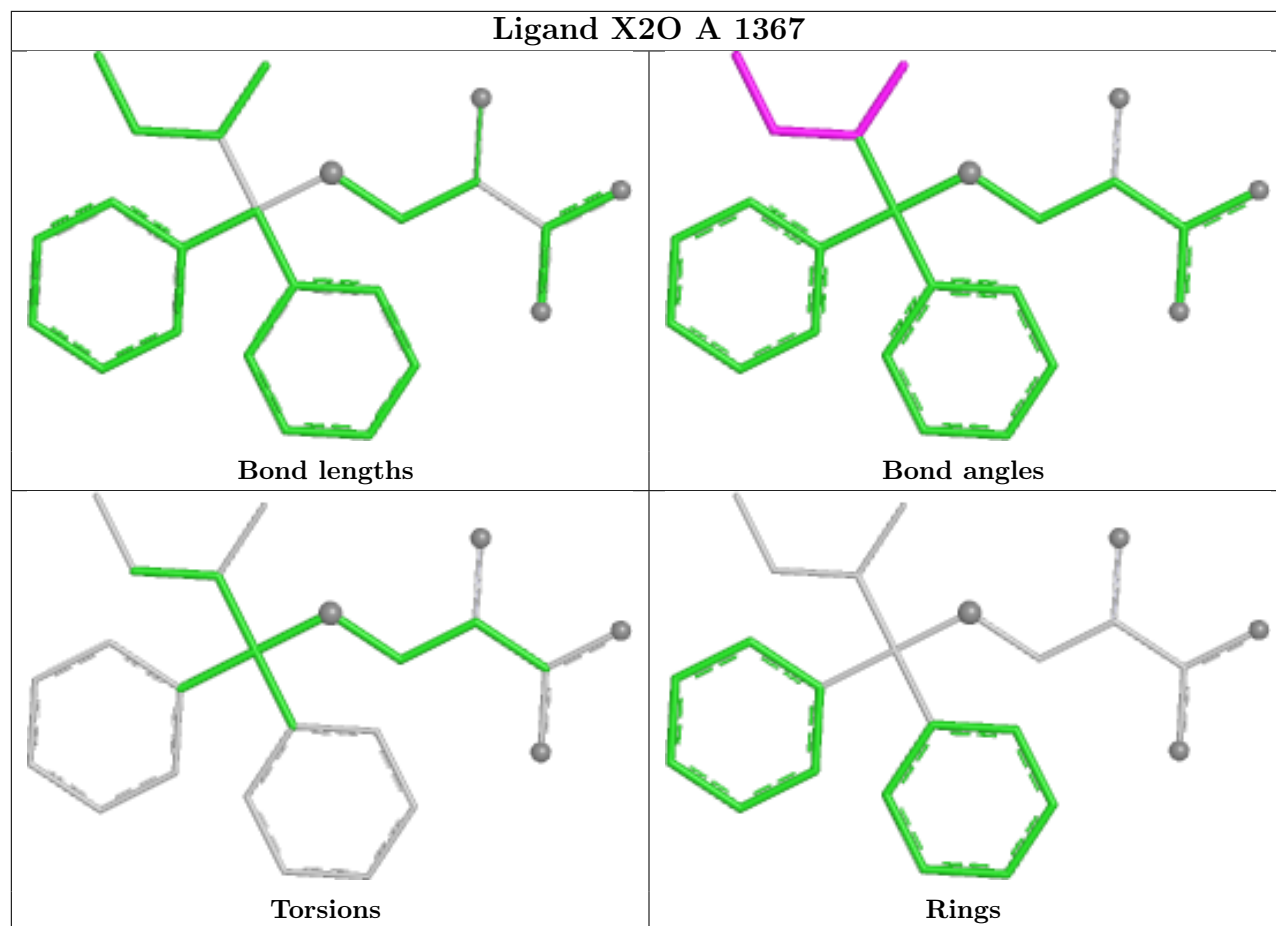


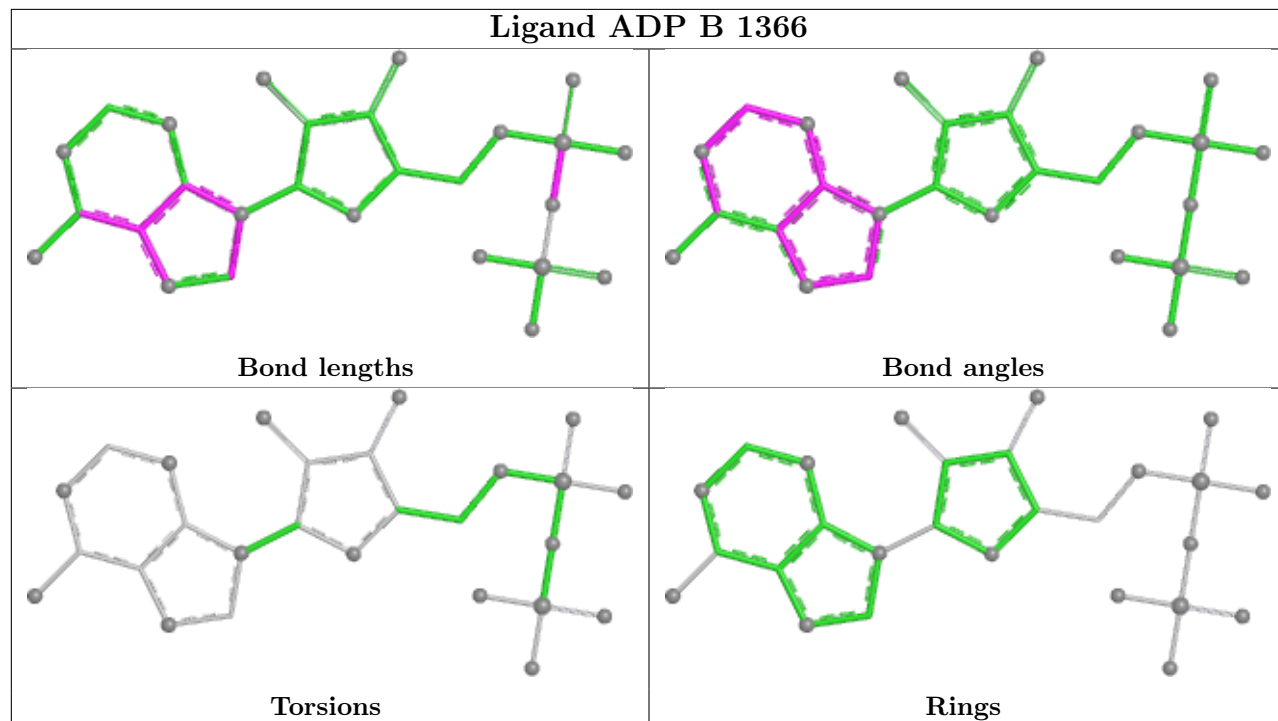
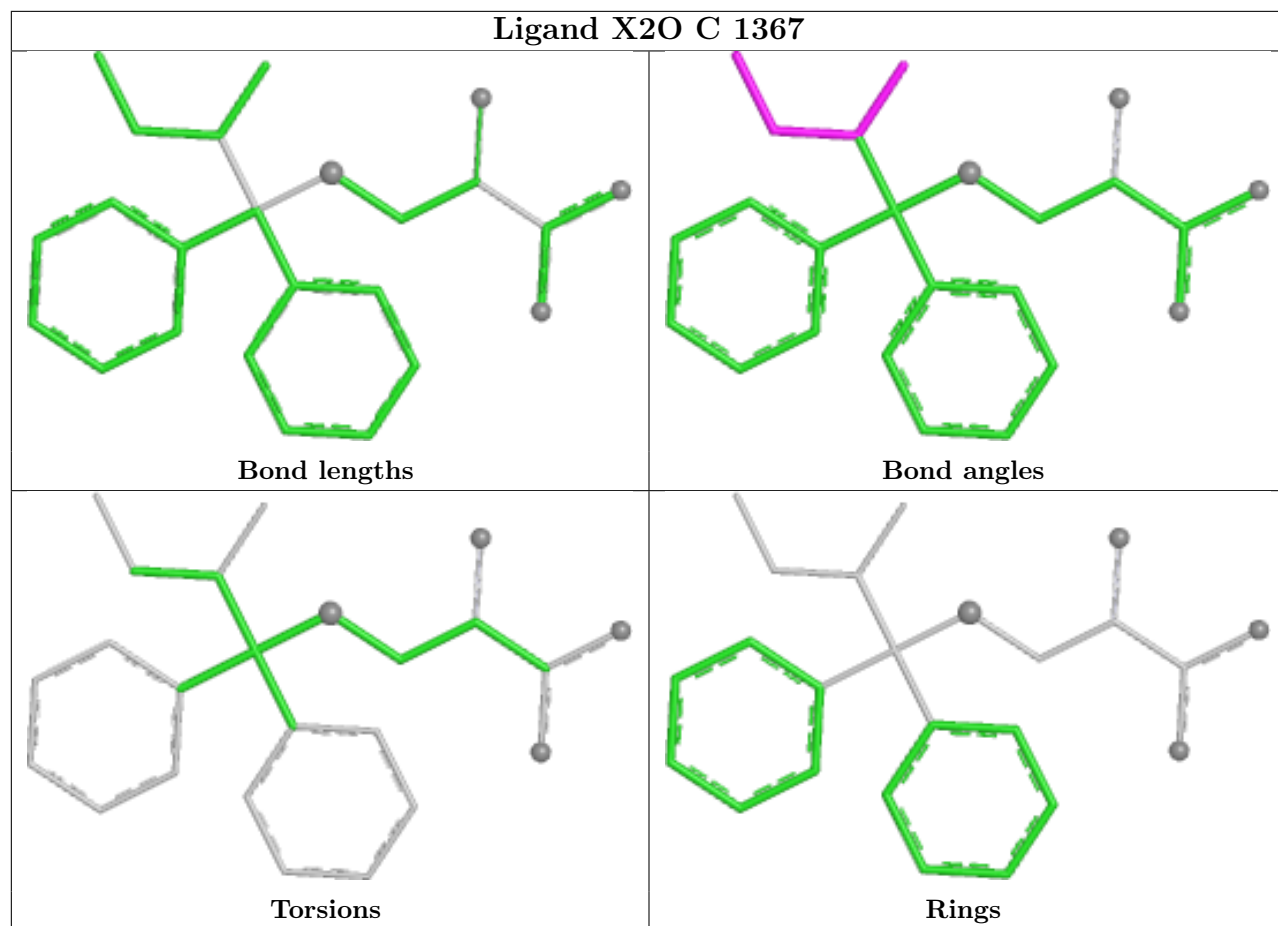
Ligand X2O B 1367



Ligand ADP A 1366







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/368 (89%)	-0.35	9 (2%) 56 53	12, 30, 69, 131	5 (1%)
1	B	324/368 (88%)	-0.41	8 (2%) 58 55	14, 29, 67, 89	10 (3%)
1	C	329/368 (89%)	0.05	9 (2%) 56 53	19, 41, 72, 97	4 (1%)
All	All	984/1104 (89%)	-0.24	26 (2%) 57 54	12, 33, 70, 131	19 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	271	ASN	4.4
1	A	365	VAL	4.2
1	C	363	PRO	3.6
1	C	255	LEU	3.6
1	A	250	ILE	3.5
1	C	327	ARG	3.5
1	B	149	ASP	3.5
1	C	304	GLU	3.3
1	B	363	PRO	3.3
1	B	247	GLU	3.1
1	B	255	LEU	3.0
1	B	248	THR	3.0
1	B	249	THR	2.8
1	B	362	LYS	2.8
1	A	248	THR	2.7
1	A	151	GLY	2.6
1	C	307	PRO	2.6
1	A	149	ASP	2.6
1	C	306	THR	2.5
1	A	152	THR	2.4
1	A	362	LYS	2.4
1	A	363	PRO	2.4
1	A	308	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	308	HIS	2.3
1	C	326	GLY	2.2
1	C	308	HIS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

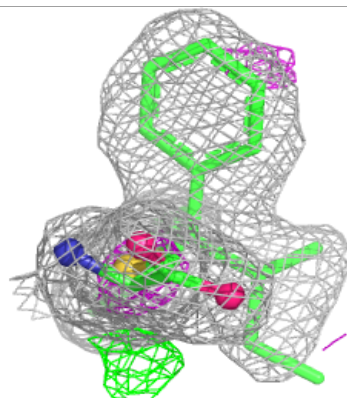
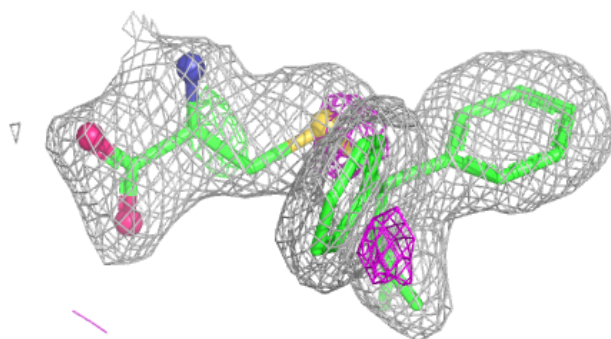
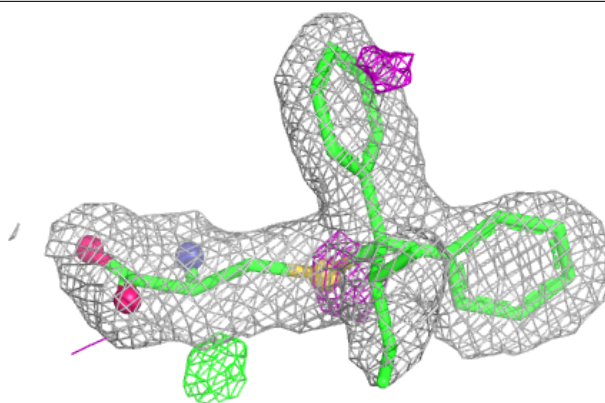
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	X2O	C	1367	24/24	0.94	0.08	27,36,40,54	0
3	X2O	B	1367	24/24	0.96	0.07	18,22,31,33	0
3	X2O	A	1367	24/24	0.96	0.07	21,30,36,43	0
4	MG	A	1368	1/1	0.96	0.09	23,23,23,23	0
4	MG	C	1368	1/1	0.96	0.10	37,37,37,37	0
4	MG	B	1368	1/1	0.98	0.06	22,22,22,22	0
2	ADP	C	1366	27/27	0.98	0.06	23,32,37,39	0
2	ADP	B	1366	27/27	0.99	0.04	16,21,27,33	0
2	ADP	A	1366	27/27	0.99	0.04	16,21,27,30	0

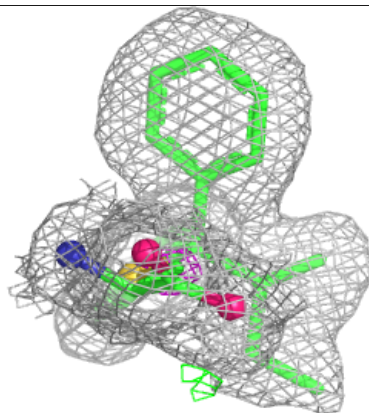
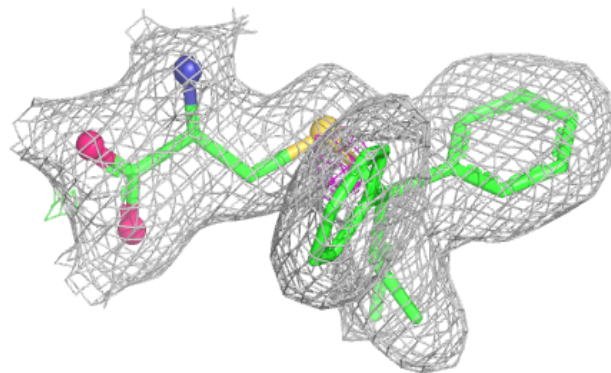
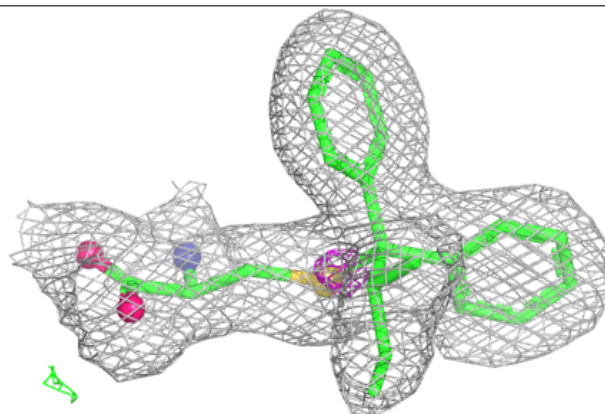
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around X2O C 1367:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

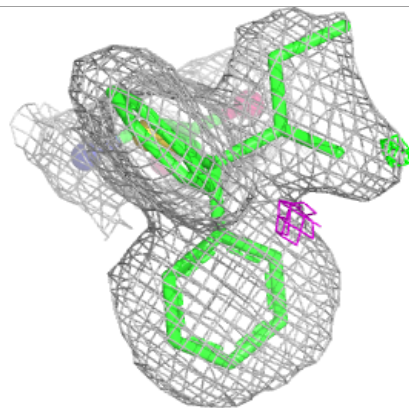
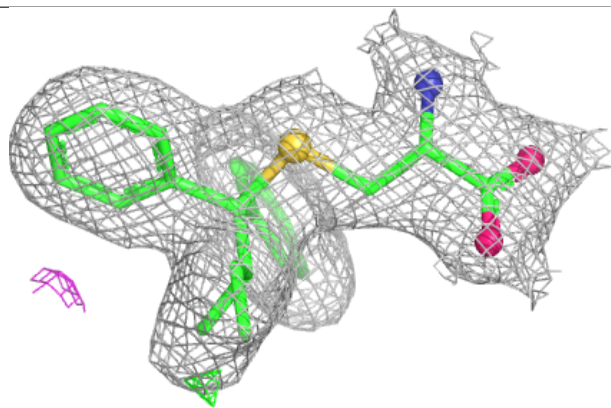
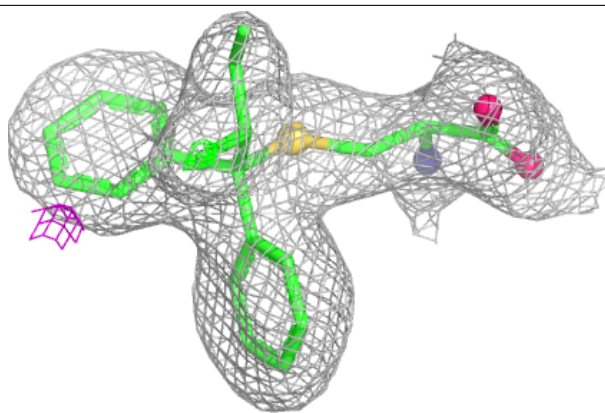
**Electron density around X2O B 1367:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



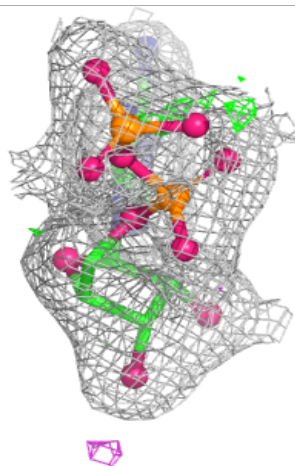
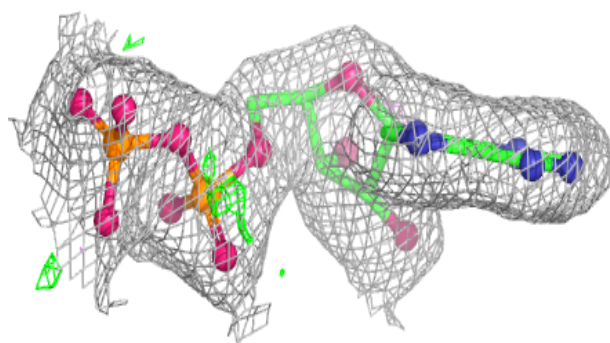
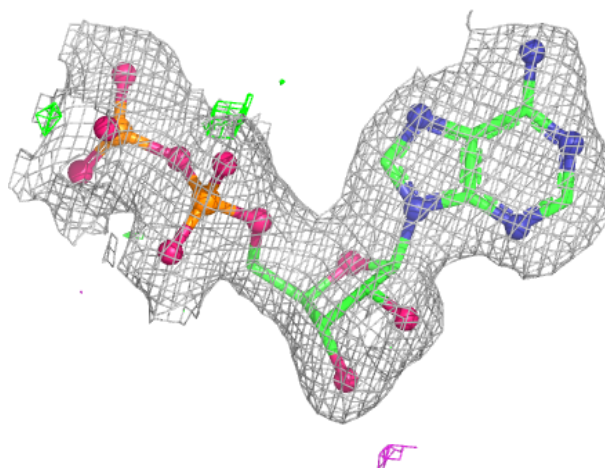
Electron density around X2O A 1367:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



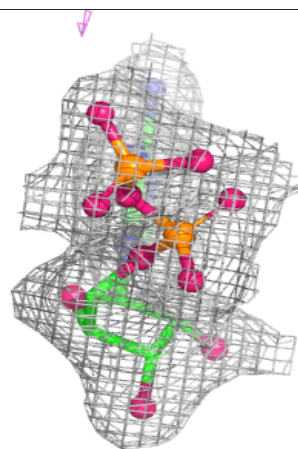
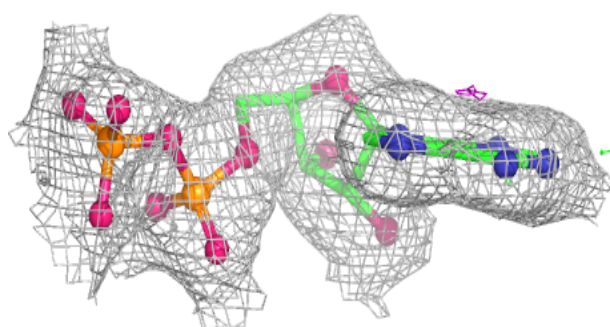
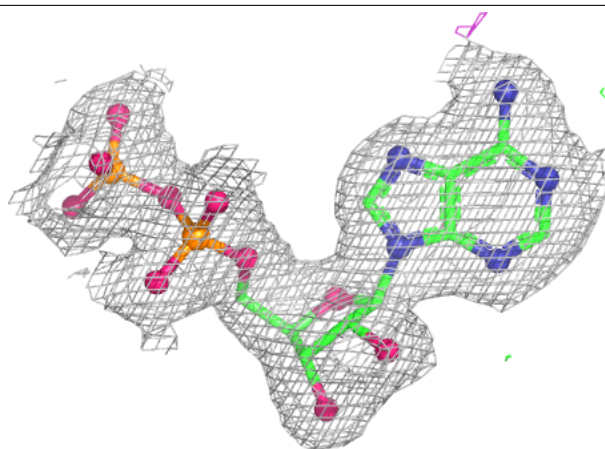
Electron density around ADP C 1366:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

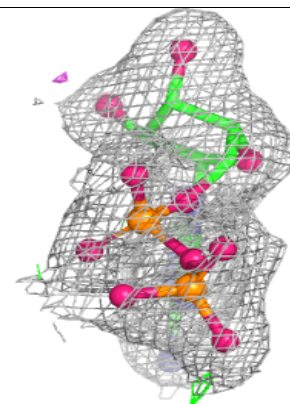
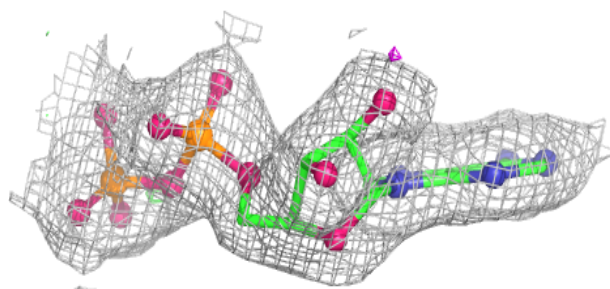
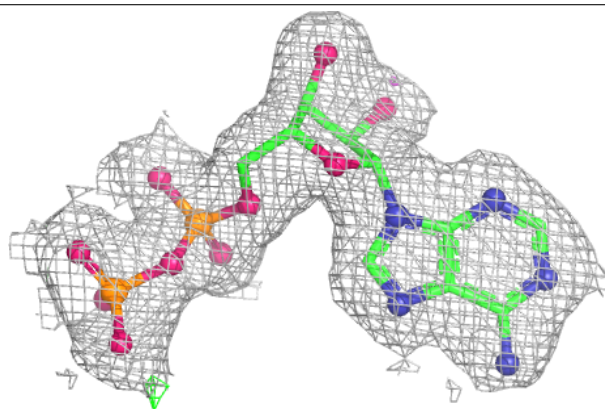


Electron density around ADP B 1366:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP A 1366:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.